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Citation for final published version:

Hasenfratz, A.P., Schiebel, R., Thornalley, D.J.R., Schonfeld, J., Jaccard, S.L., Martinez-Garcia, A., Holbourn, A., Jennings, A.E., Kuhnt, W., Lear, Caroline ORCID: <https://orcid.org/0000-0002-7533-4430>, Marchitto, T.M., Quillmann, U., Rosenthal, Y., Yu, J. and Haug, G.H. 2017. Mg/Ca-temperature calibration for the benthic foraminifera *Melonis barleeanum* and *Melonis pompilioides*. *Geochimica et Cosmochimica Acta* 217 , pp. 365-383.
10.1016/j.gca.2017.08.038 file

Publishers page: <http://dx.doi.org/10.1016/j.gca.2017.08.038>
<<http://dx.doi.org/10.1016/j.gca.2017.08.038>>

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Accepted Manuscript

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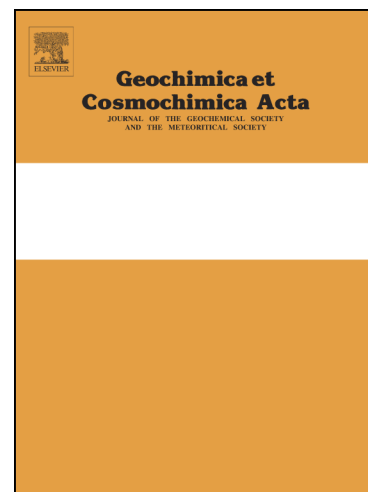
PII: S0016-7037(17)30540-9
DOI: <http://dx.doi.org/10.1016/j.gca.2017.08.038>
Reference: GCA 10443

To appear in: *Geochimica et Cosmochimica Acta*

Received Date: 16 January 2017

Please cite this article as: Hasenfratz, A.P., Schiebel, R., Thornalley, D.J.R., Schönfeld, J., Jaccard, S.L., Martínez-García, A., Holbourn, A., Jennings, A.E., Kuhnt, W., Lear, C.H., Marchitto, T.M., Quillmann, U., Rosenthal, Y., Yu, J., Haug, G.H., Mg/Ca-temperature calibration for the benthic foraminifera *Melonis barleeanum* and *Melonis pompilioides*, *Geochimica et Cosmochimica Acta* (2017), doi: <http://dx.doi.org/10.1016/j.gca.2017.08.038>

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Mg/Ca-temperature calibration for the benthic foraminifera *Melonis barleeaanum* and *Melonis pompilioides*

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Abstract

An important tool for deep-sea temperature reconstruction is Mg/Ca paleothermometry applied to benthic foraminifera. Foraminifera of the genus *Melonis* appear to be promising candidates for temperature reconstructions due to their wide geographical and bathymetric distribution, and their infaunal habitat, which was suggested to reduce secondary effects from carbonate ion saturation ($\Delta[\text{CO}_3^{2-}]$). Here, we make substantial advances to previous calibration efforts and present new multi-lab Mg/Ca data for *Melonis barleeanum* and *Melonis pompilioides* from more than one hundred core top samples spanning *in situ* bottom temperatures from -1 to 16°C , coupled with morphometric analyses of the foraminifer tests. Both species and their morphotypes seem to have a similar response of Mg/Ca to growth temperature. Compilation of new and previously published data reveals a linear dependence of temperature on Mg/Ca, with a best fit of $\text{Mg/Ca (mmol/mol)} = 0.113 \pm 0.005 * \text{BWT } (^\circ\text{C}) + 0.792 \pm 0.036$ ($r^2 = 0.81$; $n=120$; 1σ SD). Salinity, bottom water $\Delta[\text{CO}_3^{2-}]$, and varying morphotypes have no apparent effect on the Mg/Ca-temperature relationship, but pore water $\Delta[\text{CO}_3^{2-}]$ might have had an influence on some of the samples from the tropical Atlantic.

1. INTRODUCTION

Subsurface temperature reconstructions in the high latitudes are critical to an assessment of changes in paleocirculation, density stratification, and ice volume, with high latitude regions such as the Nordic Seas and the Southern Ocean being of particular importance (e.g., Elderfield et al., 2012, Ezat et al., 2014, Roberts et al., 2016). The oxygen isotopic composition of benthic foraminifer tests ($\delta^{18}\text{O}_\text{C}$) is often used in high-latitude paleoceanography (e.g., Dokken and Jansen, 1999; Bach and Bauch, 2001; Waelbroeck et al., 2002; Meland et al., 2008; Thornalley et al., 2010), but its interpretation is hindered by the multiple influences on $\delta^{18}\text{O}_\text{C}$. Mg/Ca paleothermometry applied on benthic foraminifera can be used to constrain calcification temperatures owing to the temperature-dependent

partitioning of Mg during calcification (Nürnberg et al., 1996; Rosenthal et al., 1997). Many Mg/Ca-temperature calibrations have been conducted on epifaunal *Cibicidoides* species (e.g., Lear et al., 2002; Marchitto et al., 2007; Lo Giudice Capelli et al., 2015), but the sensitivity of epifaunal Mg/Ca to temperature has recently been questioned for low temperatures (typical of high-latitudes and the deep ocean) due to the carbonate ion saturation ($\Delta[\text{CO}_3^{2-}]$) effect (Elderfield et al., 2006; Yu and Elderfield, 2008). As pore water $[\text{CO}_3^{2-}]$ has been shown to equilibrate with CaCO_3 at shallow depths within the sediment (Martin and Sayles, 1996; 2006), it has been suggested that infaunal benthic foraminifera calcifying in the surface sediment would be expected to show a weaker relationship with $\Delta[\text{CO}_3^{2-}]$ than epifaunal species (Elderfield et al., 2006; 2010). In the paleoceanographically important high-latitude regions, species of the cosmopolitan genus *Melonis* are often one of the dominant infaunal foraminifera, such as in the Nordic Seas (Belanger and Streeter, 1980; Mackensen et al., 1985), the northern North Atlantic (Thornalley et al., 2010), and the Southern Ocean (Mackensen et al., 1993; Mackensen et al., 1995).

The two existing, independent *Melonis* Mg/Ca-temperature calibrations suffer from significant uncertainties in their robustness and fidelity. The calibration of Lear et al. (2002) (0.8–18.4°C) is primarily based on samples from the Little Bahama Bank (LBB) that are very likely affected by high-Mg calcite overgrowth (e.g., Marchitto et al., 2007; Regenberg et al., 2007; Curry and Marchitto, 2008), whereas the Kristjansdottir et al. (2007) calibration (−0.2–7.0°C) is limited to core top samples retrieved from the shallow Iceland Shelf and a single sample from the Greenland margin, where seasonal and annual temperature fluctuations can amount to more than 5°C (Malmberg and Jonsson, 1997; Kristjansdottir et al., 2007), increasing uncertainty in the calcification temperature that should be used for calibration. Here, we present new multi-lab Mg/Ca data for *M. barleeianum* and *M. pompilioides* based on more than one hundred core top samples that span a wide geographic area, including bottom water temperatures from −0.9°C to 15.6°C. We evaluate the effect of salinity, bottom water $\Delta[\text{CO}_3^{2-}]$ and different morphotypes on the Mg/Ca values of *Melonis*

spp. We finally propose a new Mg/Ca-temperature calibration based on the new data as well as published data.

2. MATERIALS AND METHODS

2.1 Taxonomy and depth habitat of *Melonis*

The discrimination of extant *Melonis* species is mainly based on the spiral height of the test and the number of chambers per whorl. Due to intraspecific variability in test morphology including regional differences, probably caused by ecophenotypes, the identification of different *Melonis* species is not unequivocal (Boltovskoy, 1958; Berggren et al., 1976; Wright, 1978; Corliss, 1979; Mead, 1985; van Morkhoven et al., 1986; Thies, 1991; Mackensen et al., 1993; Bergamin et al., 1997; Milker and Schmiedl, 2012; Holbourn et al., 2013). Several *Melonis* species are considered as conspecific to the two most widely used species *M. barleeaanum* (or *M. barleeaanus*) and *M. pompilioides* (e.g., Boltovskoy, 1958; van Morkhoven et al., 1986) (Fig. 1). The rather compressed test of *M. barleeaanum* (Williamson 1858) has approximately 10–12 moderately inflated chambers that gradually increase in size (Holbourn et al., 2013). *Melonis zaandami* (Voorthuysen 1952) is considered as younger synonym of *M. barleeaanum* (Lutze et al., 1979; van Morkhoven, 1986; Thies, 1991; Schiebel, 1992; Mackensen et al., 1993; Jones, 1994; Altenbach et al., 1999). The name *M. affinis* (Reuss 1851) should be used for Paleogene species only, because their type level is Oligocene (Holbourn et al., 2013). The more spherical test of *M. pompilioides* (Fichtel and Moll 1798) has approximately 8–12 chambers that are strongly inflated and increase considerably in size and width during ontogeny (Holbourn et al., 2013). The deep-water form *M. sphaeroides* (Voloshinova 1958) is morphologically very similar to *M. pompilioides* and, by some authors, is considered an ecophenotype of *M. pompilioides* rather than a distinct species (van Morkhoven et al., 1986; Jones, 1994; Berggren and Kaminski, 1990; Holbourn et al., 2013). Furthermore, *M. soldanii* (d'Orbigny 1846) and *M. parkerae* (Uchio 1960) are considered as junior synonyms of *M. pompilioides* (Boltovskoy, 1958; Berggren et al., 1976; Mead, 1985; van Morkhoven et al., 1986). The depth distribution of infaunal *M. barleeaanum* is affected by

oxygen availability, redox boundaries, and food sources, and is largely limited to the upper 3 cm within the mesobathyal ocean floor (e.g., Jorissen et al. 1998; Fontanier et al., 2002; 2006; Schmiedl and Mackensen, 2006), although they can be occasionally found deeper in the sediment (Schumacher, 2001). Furthermore, the species is known to migrate to the sediment surface during times of low food availability (Linke and Lutze, 1993; Schönfeld, 2001). There are not many studies on the depth distribution of the usually less abundant *M. pompilioides* that was found to prefer an infaunal depth habitat closer to the surface (~0–1 cm) in the South Atlantic (Schumacher, 2001).

2.2 Sampling strategy

This work focuses on samples from several independent studies. A first group of 95 surface samples, curated at the Institute of Geosciences, University of Kiel, was collected from the Eastern North Atlantic Ocean on various cruises within the framework of the North to South Atlantic Ocean Foraminiferal Transects (NOSOFO) project (Table 1, Fig. 2). The selection of the NOSOFO surface sediment samples for this study was based on previous work on living benthic foraminiferal assemblages (Seiler, 1975; Haake, 1980; Lutze and Coulbourn, 1984; Mackensen et al., 1985; Thies, 1991; Timm, 1992; Schiebel, 1992; Altenbach et al., 1999; Altenbach et al., 2003; Schönfeld and Altenbach, 2005). *Melonis* specimens from these samples, together with one Pacific Southern Ocean core top, were morphometrically analyzed at the Department of Climate Geochemistry, Max Planck Institute for Chemistry (MPIC), and their geochemical composition was measured at the Geological Institute, ETH Zurich (ETHZ). A second supplementary set of core top samples from high sedimentation rate cores in the subpolar North Atlantic were utilized, with samples from 11 core sites cleaned and measured at the School of Earth and Ocean Sciences, Cardiff University (CU), samples from a further two core sites analyzed at the Godwin Laboratory for Palaeoclimatic Research, Department of Earth Sciences, University of Cambridge (GLPR), and one surface sediment sample analyzed at the Institute of Arctic and Alpine Research, University of Colorado (INSTAAR). Another five core tops were retrieved from the Oslofjord (Risdal, 1964) and also

processed at INSTAAR. Three additional samples were obtained from the Sulawesi margins in Indonesia and analyzed at CU. Finally, one core top sample from the eastern South Atlantic was processed at the Department of Earth Sciences, University of Bristol (UoB). Overall, the core top sediments span a wide latitudinal range from the tropics to polar realms and were retrieved from water depths ranging between 50 and 4305 m (Table 1, Fig. 2).

2.3 Analytical techniques at MPIC and ETHZ

Depending on the abundance of *Melonis* (Table 1), a varying number of dead individuals (13 ± 6 individuals, $255 \pm 127 \mu\text{g}$) was picked from the $>250 \mu\text{m}$ size range at the Institute of Geosciences, University of Kiel. In order to allow a clear distinction between the compressed *M. barleea* and the inflated *M. pompilioides*, morphometric analyses of the foraminifer tests were carried out at MPIC. Tests were photographed using an Olympus SZX16 binocular incident light microscope with a planapochromatic objective, equipped with an Olympus UC90 digital camera (image resolution of $1.32 \times 1.32 \mu\text{m}$ per pixel). All individuals were photographed from the side in order to allow counting of chambers. Well-preserved representatives of compressed to spherical morphotypes from all samples, i.e. a total of 452 tests, were photographed in frontal view in order to determine the aspect ratio (AR). The AR of the foraminifer test denotes the ratio between spiral height (maximum test diameter) and spiral width (maximum test diameter perpendicular to the plane of symmetry of the planispiral tests) (see Fig. 3a), and was determined in an automated way using the image analysis software Olympus Stream Essentials version 2.1.

Following the morphometric analyses, samples were cleaned and analyzed for trace metals at ETHZ. The cleaning procedure applied is that published by Barker et al. (2003), i.e. omitting the reductive cleaning step (Boyle and Keigwin, 1985) that has been shown to lower the Mg/Ca ratio of the remaining biogenic carbonate (Martin and Lea, 2002; Barker et al., 2003; Rosenthal et al., 2004; Elderfield et al., 2006; Yu et al., 2007; Yu and Elderfield, 2008; Bian and Martin, 2010; Hasenfratz et al., 2017). Prior to cleaning, foraminifer tests were weighed

and gently crushed between two glass plates under a microscope to allow contaminant phases to be removed during cleaning (Boyle and Keigwin, 1985). If enough material was present, the crushed material was split into two subsamples to allow duplicate measurements. Element/Ca ratios of the cleaned foraminifera material were measured by ICP-MS at ETHZ using a single collector, high-resolution magnetic-sector Thermo Scientific Element XR instrument (see Hasenfratz et al., 2017 for details in cleaning and measuring procedures). The primary standard has been prepared at ETHZ and has a Mg/Ca ratio of 5.59 mmol/mol. The six consistency standards, prepared at the University of Bristol and the University of Cambridge (CL2, CL3, CL4, and CL9; Greaves, 2008), have a composition similar to foraminiferal carbonate (0.51–3.29 mmol/mol of Mg/Ca). They have been measured regularly between August 2014 and August 2016 and are on average within 1.4 % (2 SD; standard deviation) of the gravimetric value for Mg/Ca, with an average long-term reproducibility of ± 2.8 % (2 RSD; relative standard deviation). Duplicate measurements obtained for 36 *Melonis* core top samples, split after crushing and mixing, and before cleaning, show a good reproducibility with 2 SD and 2 RSD of 0.06 mmol/mol and ± 4.2 %, respectively.

Al/Ca, Mn/Ca, and Fe/Mg are used to check for cleaning efficiency (Barker et al., 2003). Contamination is indicated by Mn/Ca higher than 0.25 mmol/mol, which would increase shell Mg/Ca by around ~ 0.05 mmol/mol and inferred Mg/Ca-temperatures by $\sim 0.5^{\circ}\text{C}$, given Mg/Mn ratios in foraminiferal coatings of ~ 0.2 and a typical Mg/Ca temperature sensitivity of ~ 0.1 mmol/mol per $^{\circ}\text{C}$ in infaunal benthic foraminifera (Elderfield et al., 2012; Hasenfratz et al., 2017). Moreover, samples with Fe/Ca and Fe/Mg higher than 0.25 mmol/mol and Al/Ca values higher than 0.5 mmol/mol, respectively, were rejected due to potential silicate contamination (Table 1).

2.4 Analytical techniques at the other laboratories

Foraminiferal samples have been cleaned oxidatively (Barker et al., 2003) at GPRL and UoB, and including the reductive step (Boyle and Keigwin, 1985) at INSTAAR. At CU, both

approaches were used. Trace metal analysis was performed on a Perkin-Elmer Elan DRC II quadrupole ICP-MS at GLPR (Yu et al., 2005), on a Thermo Finnigan Element 2 ICP-MS at UoB (Rae et al., 2011) and INSTAAR (Marchitto, 2006), and on a Thermo Element XR ICP-MS at CU (Lear et al., 2002, 2010). The long-term precision on Mg/Ca is 1.1 % at INSTAAR, better than 2 % at UoB, and ~2 % at CU and GPRL (2 RSD). Interlaboratory comparisons indicated that the five laboratories ETHZ, GPRL, UoB, INSTAAR and CU agree well with each other. The consistency standards from GPRL and UoB that have been regularly measured at ETHZ are on average within 1.5 % (2 RSD; GPRL) and 1.1 % (2 RSD; UoB) of the gravimetric value for Mg/Ca, indicating that these three laboratories are consistent with each other. GPRL and INSTAAR have both participated in the interlaboratory study from Greaves et al. (2008), with an average offset of 1.4 % (2 RSD). Furthermore, measurement of standards at GPRL and CU indicated that the laboratories in Cambridge and Cardiff agree with each other within analytical error.

Potentially contaminated data were rejected using the same thresholds as noted above (Table 1). The aspect ratio of the *M. barleeianum* specimens was not quantitatively determined, but the compressed and inflated morphotypes were treated individually at INSTAAR.

2.5 Hydrographic data

Annual averaged bottom water temperature (BWT) (Locarnini et al., 2013) and salinity (Zweng et al., 2013) values for the core top sites were retrieved from World Ocean Atlas 2013 (WOA13) version 2 (0.25° grid resolution; 1955–2012). Bottom water $\Delta[\text{CO}_3^{2-}]$ was estimated using total CO_2 and total alkalinity (ALK) from the 1° grid resolution dataset provided by Goyet et al. (2000). $[\text{CO}_3^{2-}]$ and the saturation state for calcite (Ω) were calculated using CO2calc version 1.3.0 (Robbins et al., 2010), with the dissociation constants K_1 and K_2 as defined by Mehrbach et al. (1973) and refit by Dickson and Millero (1987). The carbonate saturation concentration $[\text{CO}_3^{2-}]_{\text{sat}}$ was calculated by $[\text{CO}_3^{2-}]/\Omega$, and the degree of saturation ($\Delta[\text{CO}_3^{2-}]$) was obtained by the difference between $[\text{CO}_3^{2-}]$ and $[\text{CO}_3^{2-}]_{\text{sat}}$. The

estimated bottom water temperature, salinity and bottom water $\Delta[\text{CO}_3^{2-}]$ at the core top sites used in this study range between -0.9°C and 15.6°C , 34.4 and 36.3 psu, and -2 and $122\ \mu\text{mol/kg}$, respectively (Table 1).

3. RESULTS

3.1 Morphometric differentiation of *Melonis* species

Averages of ARs and number of chambers for each of the core top samples show a bimodal distribution of two distinctively different *Melonis* morphotypes (Fig. 3), with the smaller group having lower AR (~ 1.1 – 1.5 ; spherical type) and a larger group including more compressed tests with higher and more variable ARs (~ 1.5 – 2.8). The specimens within the larger group, with an average chamber number of 11.2 ± 1.0 , are assigned to *M. barleeaanum*. Despite the wide intraspecific range of ARs within *M. barleeaanum*, the distribution is nearly Gaussian with a continuous change from relatively inflated to more compressed subtypes. A similar or even larger variability in the AR of *M. barleeaanum* was observed by Bergamin et al. (1997) in the Mediterranean Sea (~ 1.6 – 2.5), and by Thies (1991) in the North Atlantic (~ 1.6 – 3.8), respectively. Secondly, the strongly inflated specimens within the smaller group have an average of 7.2 ± 0.7 chambers in the final whorl. These specimens were collected from water depths of 2000 to 4300 m (Fig. 2). The lesser number of chambers and the occurrence in abyssal depths, together with the low AR, characterize the abyssal plain-inhabiting ecophenotype of *M. pompilioides* (e.g., Holbourn et al., 2013).

3.2 Mg/Ca in *Melonis*

Following Yu et al. (2007), who found a significant linear correlation between Mg/Ca values resulting from oxidative and reductive cleaning, Mg/Ca values derived from reductively cleaned benthic foraminifera tests are corrected (increased) by a factor of 1.10. Mg/Ca values in *M. barleeaanum* range between 0.68 and 2.74 mmol/mol (Fig. 4a) over sites with BWT of -0.9°C to 15.6°C (Table 1). As *M. pompilioides* has only been found in deep water samples at BWT of 0.8 – 3.5°C (Fig. 2), their Mg/Ca is confined to values of 0.81–1.06 mmol/mol. From

131 analyzed samples, 6 samples were rejected due to potential contamination indicated by elevated Mn/Ca, Fe/Ca, Fe/Mg, and Al/Ca ratios (Table 1). No offset (0.003 ± 0.087 mmol/mol) was found between compressed and inflated *M. barleeaanum* co-occurring in three samples (Oslofjord, station 6; GIK8060; GIK16005). A small offset (0.08 ± 0.20 mmol/mol) can be observed between sympatric *M. barleeaanum* and *M. pompilioides* measured in five samples (GIK16906, GIK12328, GIK13533, GIK12347, GIK13238), but this offset vanishes if sample GIK13238 (offset of 0.40 mmol/mol) is removed from the statistics (0.01 ± 0.11 mmol/mol) (see also Table 1). The limited number of samples with sympatric *Melonis* specimens of varying morphometry (AR and number of chambers) impedes statistically safe statements on the intra- and interspecific variability of *Melonis*. However, the relatively small Mg/Ca offsets suggest that foraminifera of the genus *Melonis* have a similar temperature response. In general, Mg/Ca ratios and BWT of *Melonis* are relatively well related to each other, defining a linear positive relationship (Fig. 4a).

4. DISCUSSION

4.1 Comparison to published *Melonis* Mg/Ca data

Fig. 4b presents a compilation of *Melonis* Mg/Ca core top data, including data presented in this study and published data from the Norwegian Sea and the Greenland and Iceland shelf (Elderfield et al., 2006; Kristjansdottir et al., 2007; Ezat et al., 2014), the North Atlantic (Lear et al., 2002; Tachikawa and Elderfield, 2004; Marcott et al., 2011), the Bahama Banks, the Gulf of California, and the Pacific Southern Ocean (Lear et al., 2002). For consistency, the Mg/Ca data derived from the full cleaning procedure are corrected by a factor of 1.10 (Yu et al., 2007), and the BWT information is taken from WOA13 for all locations for which Mg/Ca data are presented. As suggested by many studies, the Mg/Ca data from shallow, carbonate-rich sediments of the LBB are not considered in this study as they are very likely contaminated by secondary high-Mg coatings (Reuning et al., 2005; Elderfield et al., 2006; Rosenthal et al., 2006; Marchitto et al., 2007; Regenberg et al., 2007; Curry and Marchitto, 2008; Lear et al., 2008) (see open pink circles in Fig. 4b).

With a few exceptions (Table 1), most of the Mg/Ca data were measured on core top material from the eastern North Atlantic, encompassing the entire latitudinal range from the tropical to the polar realms. Despite the close relationship between Mg/Ca and temperature, the scatter around the linear fit appears to be non-random, with the tropical eastern Atlantic data mostly falling below the regression line (Figs. 4c, 5). As all the tropical Atlantic samples and the majority of the other samples were cleaned oxidatively (Table 1), it is unlikely that their Mg/Ca values were biased during cleaning. Also, like the majority of the samples, they were cleaned at ETH. Furthermore, we can exclude a bias from selected BWT, as *in situ* temperatures measured directly above the core sites of the Gulf of Guinea samples (Lutze et al., 1988) compare very well with the WOA13 temperatures, the latter of which are on average only 0.14°C higher than the former ($r^2 = 0.98$; $p = 4.8 \times 10^{-23}$; $n = 27$). In order to further assess the possible cause of variability in the Mg/Ca-BWT relationship, the potential influences on the standardized Mg/Ca residuals are discussed in the following sections.

4.2 Evaluation of the influence of salinity, $\Delta[\text{CO}_3^{2-}]$, and morphotype

Bottom water temperature, salinity, and $\Delta[\text{CO}_3^{2-}]$ tend to covary over large parts of the deep ocean, generally decreasing with depth. Although it is widely accepted that temperature is the primary control on foraminiferal Mg/Ca, changes in salinity were shown to have a significant effect on planktonic Mg/Ca ratios (e.g., Nürnberg et al., 1996; Ferguson et al., 2008; Hönisch et al., 2013). However, the influence of salinity on benthic foraminifera is debated. While most of the culture (e.g., Toyofuku et al., 2000; Diz et al., 2012) and calibration studies (e.g., Weldeab et al., 2016) have found no salinity effect, an alternative experiment revealed an increase of 3.2–3.6 % in benthic Mg/Ca per salinity unit (Dissard et al., 2010). Bottom water salinity at the sites discussed here (Table 1) ranges from 34.4 to 36.4 psu, but there is no evidence of an influence on the foraminiferal Mg/Ca residuals, when all data are considered ($r^2 = 0.02$; $p = 0.07$; $n = 154$) (Fig. 6a). However, the samples from the eastern tropical Atlantic show a positive correlation between Mg/Ca residual and salinity over a small salinity

range of 0.5 psu ($r^2 = 0.40$; $p = 4.8 \times 10^{-5}$; $n = 35$), indicating that salinity might have an influence on the variability observed in the eastern tropical Atlantic data (Fig. 6a).

During the past decade, several studies proposed that bottom water $[\text{CO}_3^{2-}]$ affects the incorporation of Mg into epibenthic foraminiferal test carbonate, with lower Mg/Ca ratios in both undersaturated and strongly oversaturated conditions (Rosenthal et al., 2006; Elderfield et al., 2006; Marchitto et al., 2007; Yu and Elderfield, 2008; Lear et al., 2010). The influence of $[\text{CO}_3^{2-}]$ on infaunal benthic foraminifera is yet poorly constrained and has been appraised differently. The major uncertainty appears to reside in the estimation of the pore water $\Delta[\text{CO}_3^{2-}]$ within the shallow sediment depth the foraminifera are living in. Elderfield et al. (2006; 2010) assumed that the $\Delta[\text{CO}_3^{2-}]$ effect weakens with increasing habitat depth in the sediment, based on pore water sampling that indicated rapid equilibration of pore water $[\text{CO}_3^{2-}]$ with CaCO_3 within the first few centimeters (Martin and Sayles, 1996; 2006). In their view, infaunal foraminifera living a few centimeters below the sediment surface would not be expected to show a $\Delta[\text{CO}_3^{2-}]$ effect. This hypothesis has been recently challenged by Weldeab et al. (2016) who have used total alkalinity and pH measurements in pore water from Atlantic sediments (1–10 cm) to show that pore water $\Delta[\text{CO}_3^{2-}]$ is lower by about 40–50 $\mu\text{mol/kg}$ compared to the overlying bottom water $\Delta[\text{CO}_3^{2-}]$, independently of the saturation state of the overlying bottom waters.

Due to the linear correlation between bottom water and pore water $\Delta[\text{CO}_3^{2-}]$ (Weldeab et al., 2016), the bottom water $\Delta[\text{CO}_3^{2-}]$ estimates can be used to evaluate the $\Delta[\text{CO}_3^{2-}]$ effect on the Mg/Ca ratios of the infaunal foraminifera. Multiple observations indicate that there is likely no systematic effect of $\Delta[\text{CO}_3^{2-}]$ on the Mg/Ca ratios of the infaunal *Melonis*. First, Mg/Ca residuals seem to vary independently from their corresponding $\Delta[\text{CO}_3^{2-}]$, even at the lowest bottom water $\Delta[\text{CO}_3^{2-}]$ values ($r^2 = 0.05$; $p = 0.004$; $n = 153$). Also, although bottom water $\Delta[\text{CO}_3^{2-}]$ is lower than 40 $\mu\text{mol/kg}$ for most of the tropical Atlantic sites (and the respective pore water $\Delta[\text{CO}_3^{2-}]$ values might even be lower; Weldeab et al., 2016), corresponding to negative Mg/Ca residuals, the overall relationship between their Mg/Ca residuals and

carbonate ion saturation is not consistent ($r^2 = 0.03$; $p = 0.33$; $n = 35$) (Fig. 6b). Secondly, in contrast to studies that have observed distinctly elevated Mg/Ca values in epifaunal *Cibicidoides* from the Nordic Seas, interpreting them as being affected by the anomalously high $\Delta[\text{CO}_3^{2-}]$ (Martin et al., 2002a; Elderfield et al., 2006; Yu and Elderfield, 2008), no significant correlation was found in the Nordic Seas samples ($r^2 = 0.07$; $p = 0.06$; $n = 51$). In fact, the Mg/Ca ratios of the 27 Nordic Seas samples that were retrieved below the thermocline (> 500 m; very stable deep water temperatures, but varying $\Delta[\text{CO}_3^{2-}]$) have very low Mg/Ca ratios of 0.82 ± 0.11 mmol/mol (Table 1). These observations corroborate the hypothesis laid out by Elderfield et al. (2006) that infaunal foraminifera, such as *Uvigerina* spp. and *Melonis* spp., might be less affected by carbonate ion saturation effects.

As discussed above, the pore water $\Delta[\text{CO}_3^{2-}]$ can deviate from that of the bottom water, which, amongst other things, depends on the primary productivity and the remineralization of organic matter within the upper sediment (e.g., Emerson et al., 1982; Martin and Sayles, 1996; Weldeab et al., 2016). In general, *M. barleeianum* has been associated with a high-productivity regime in the surface ocean (Mackensen et al., 1985; Lutze et al., 1986; Mackensen et al., 1993; Schmiedl et al., 1997; Rudolph, 2006). Their maximum abundances are centered at flux rates of 3 to 10 g C m⁻² yr⁻¹ particulate organic carbon (Altenbach et al., 1999). Information on core top organic carbon content was only available for 40 % of the core tops, including the majority of the tropical Atlantic sites (Müller, 1975; Diester-Haass and Peter, 1979; Mackensen, 1985; Lutze et al., 1986; Tiedemann, 1986; Westerhausen et al., 1993) and some of the Norwegian Sea (Mackensen et al., 1985; Hoff et al., 2016), the northern North Atlantic (Austin and Evans, 2000; Thomson et al., 2000), and the Pacific Southern Ocean sites (Wagner et al., 2013). In general, seafloor organic matter flux and total organic carbon (TOC) is higher at the northwestern African margin and the eastern equatorial Atlantic than at the other sites (Fig. 6c). Given the availability of oxygen in pore waters, remineralization of organic matter might depress pore water $\Delta[\text{CO}_3^{2-}]$ compared to the already relatively low bottom water values due to increased bacterial respiration. Interestingly, in this

study, a trend between the sedimentary TOC and the Mg/Ca residuals has been found, irrespective of the *Melonis* species (all data: $r^2 = 0.31$; $p = 2.2 \times 10^{-6}$; $n = 62$; tropical Atlantic: $r^2 = 0.17$; $p = 0.02$; $n = 33$). Although the evidence is weak, and, for instance, the lability of the organic matter is not taken into account, the negative relationship between tropical Atlantic Mg/Ca residuals and TOC might suggest that benthic foraminifera from sediments experiencing high organic matter fluxes and increased production of CO_2 by remineralizing bacteria have altered Mg/Ca ratios due to a fractionation effect during calcification in undersaturated pore waters (Martin et al., 2002b; Yu and Elderfield, 2008) or due to preferential (post-mortem) dissolution of Mg-rich parts of the carbonate (McCorkle et al., 1995; Martin et al., 2005). As the investigated *Melonis* specimens did not show any apparent dissolution features, the former scenario is more likely. Another aspect that might alter the relationship between organic matter flux and Mg/Ca residual is the change in the depth habitat of *Melonis* as *M. barleeaanum* was shown to migrate deeper in the sediment during times of increased food availability. However, because pore water $\Delta[\text{CO}_3^{2-}]$ does not show a clear decline below ~1–2 cm and remains relatively stable (Weldeab et al., 2016), we conclude that the potential vertical migration of *Melonis* spp. has a negligible influence on the $\Delta[\text{CO}_3^{2-}]$ effect.

Finally, we assessed if varying morphotypes of *M. barleeaanum* can explain some of the variation in the Mg/Ca residuals. Comprehensive, quantitative morphometric information is only available for the samples investigated at ETHZ/MPIC. In general, there is a relatively large variation in the AR within regions, but there is a tendency of more compressed types corresponding to more negative Mg/Ca residuals ($r^2 = 0.27$; $p = 1.9 \times 10^{-7}$; $n = 89$), specifically for the eastern tropical Atlantic samples ($r^2 = 0.42$; $p = 1.3 \times 10^{-4}$; $n = 29$) (Fig. 6d). As initial measurements on a small set of sympatric *M. barleeaanum* morphotypes indicated that there is probably no intraspecific offset, we suspect that the reason for this correlation is spurious. It is possible that the relationship between morphotype and Mg/Ca residual may be partly controlled by the causal connection between aspect ratio of *M.*

barleeaanum and organic matter flux (with the latter potentially affecting pore water $\Delta[\text{CO}_3^{2-}]$ as discussed above). In previous studies, it was found that more compressed morphotypes of *M. barleeaanum* are more abundant in upwelling regions such as the northwestern African margin, while the more inflated types are found predominantly in low-productivity areas or during periods of food scarcity, probably due to a link between habitus and food supply (Thies, 1991; Altenbach et al., 1993; Bhaumik et al., 2014). Although there is indeed a weak positive trend between TOC and aspect ratio of *M. barleeaanum* in our dataset ($r^2 = 0.22$; $p = 6.7 \times 10^{-4}$; $n = 49$; plot not shown), it is difficult to assess the causality between the two parameters given the limited number of samples.

In summary, the evaluation of our data indicates that bottom water $\Delta[\text{CO}_3^{2-}]$ and varying morphotype cannot explain the variability of the Mg/Ca-BWT data. However, the relatively high TOC contents in sediments below high-productive regions could be an indicator for lowered pore water $\Delta[\text{CO}_3^{2-}]$ that might provide an explanation for the relatively low Mg/Ca residuals for most of the eastern tropical Atlantic samples. In contrast to the entire dataset, there seems to be a salinity effect in the tropical Atlantic data, but the relatively narrow salinity range makes it difficult to conclusively assess its influence. Last, although we cannot exclude that the specimens from the tropical Atlantic and the other regions (Table 1) represent different cryptic species of *M. barleeaanum* and *M. pompilioides*, which respond to BWT in a differential way, the similar reaction in Mg/Ca ratios of the two *Melonis* species renders this scenario unlikely.

4.3 Calibration

In order to construct a reliable Mg/Ca-temperature calibration, it is important that all data included are robust (Fig. 4b). To ensure that the different laboratories where the data have been produced are consistent with each other, it was decided to only use data that have been newly acquired for this project (80 % of all available data on *Melonis* spp.), and all other data are used for comparison. Multiple regression analysis of these 125 data points detected four

data points whose standardized residuals are higher than $\pm 3\sigma$ (with very high Cook's distances of > 0.14 ; Cook and Weisberg, 1982), and one data point with a residual $\pm 2.6\sigma$ (Cook's D of 0.08). These outliers cannot be explained by environmental parameters, such as salinity or $\Delta[\text{CO}_3^{2-}]$. The standardized residual threshold to reject data designated for temperature calibrations varies in the literature from $\pm 1\sigma$ (e.g., Kim et al., 2008) to $\pm 3\sigma$ (e.g., Conte et al., 2006), or when Cook's D greatly exceeds $4/n$, with n being the number of samples (0.032 for this dataset) (e.g., Mackay et al., 2003). The threshold mostly used in foraminiferal Mg/Ca paleothermometry is $\pm 2\sigma$, which should comprise $\sim 95\%$ of the data (e.g., Rathmann et al., 2004; Haarmann et al., 2011; Quillmann et al., 2012). Given that the remaining 120 data all have residuals within the $\pm 1.7\sigma$ range and within 0.03 of Cook's distance, the five data points with residuals larger than $\pm 2\sigma$ (Cook's D larger than 0.08) were removed from the calibration data set in order to prevent the outliers exerting undue leverage on the final statistical estimates (see Table 1).

In contrast to previous calibrations that have found (weak) evidence for an exponential response of *Melonis* Mg/Ca to temperature (Lear et al., 2002; Kristjansdottir et al., 2007), the data are best explained by a linear relationship, with a sensitivity of 0.11 mmol/mol Mg/Ca per $^{\circ}\text{C}$ (Fig. 4d):

$$\text{Mg/Ca} = 0.113 \pm 0.005 T + 0.792 \pm 0.036 \quad (r^2 = 0.81; n = 120; 1\sigma \text{ SD}) \quad (1)$$

The calibration uncertainty increases with increasing Mg/Ca, resulting into a 1σ temperature error of $\pm 0.3^{\circ}\text{C}$ and $\pm 1.0^{\circ}\text{C}$ for temperatures around -1°C and 16°C , respectively.

In a foraminiferal Mg/Ca interlaboratory study, Rosenthal et al. (2004) showed that a large part of the variability was due to the application of different cleaning methods, concluding that a consistent protocol would improve the comparability of Mg/Ca results. The calibration dataset consists of 13 samples that have gone through the full cleaning procedure, including reductive cleaning that has been shown to decrease foraminiferal Mg/Ca values (e.g., Elderfield et al., 2006; Yu et al., 2007). In this study, we correct for this bias in benthic

Mg/Ca values using the linear fit between samples that were oxidatively and reductively cleaned, respectively, as given by Yu et al. (2007). Their comparison is based on *Cibicoides* and *Uvigerina* species, which might have a different susceptibility to the corrosive cleaning solution than *Melonis* species. The amount of Mg-enriched carbonate preferentially dissolved from the foraminifer tests depends on many factors (e.g., porosity, homogeneity of the Mg distribution, amount of coating, degree of crushing before cleaning), and the correction might introduce additional uncertainty (Quillmann et al., 2012). However, we consider that the added uncertainty is minimal. First, although the coefficient is based on three different benthic genera, their effect on the reductive cleaning is very similar ($r^2 = 0.93$) (Yu et al., 2007). Second, the effect of the reductive cleaning in the interlaboratory study from Rosenthal et al. (2004) is relatively consistent for the foraminifera used ($r^2 = 0.97$), indicating that a coefficient determined in one lab can be applied for data produced in other laboratories. Last, discarding the reductively cleaned samples would not change the sensitivity of the calibration presented in this study, resulting into a small temperature difference ($\sim 0.2\text{--}0.4\text{ }^{\circ}\text{C}$) that is within the uncertainty of the calibration. This suggests that the coefficient used to correct reductively cleaned data can also reliably be applied for *Melonis* spp.. Similarly, excluding the samples from the tropical Atlantic that might be partly biased by lowered pore water $\Delta[\text{CO}_3^{2-}]$ (or might have a salinity effect) would not affect the slope of the linear fit, but would change the intercept leading to temperature differences of $\sim 0.4\text{--}1.2\text{ }^{\circ}\text{C}$. Because the evidence of a possible bias is small, we recommend using the calibration equation that includes all the data. In Fig. 4d, the different calibration equations are compared to each other.

The previously published data (excluding the LBB samples) compare relatively well to the new data, except for five data points from the Nordic Seas (Kristjansdottir et al., 2007; Elderfield et al., 2006) that have relatively high Mg/Ca residuals (Figs. 4b, 5a). Concerning the three data points from Kristjansdottir et al. (2007), we suspect that the reason for the high residuals are temperature uncertainties, as discussed in the initial calibration study. In detail, the BWT obtained from CTD casts at the core top locations during the B997 cruise in July

1997 (Kristjansdottir et al., 2007) and temperatures sourced from WOA13 were found to differ by more than 2 °C for 4 of the 15 sites (2.87 ± 0.68 °C) on the Iceland shelf (with the three mentioned sites, 314, 315 and 337, among these four sites). Bottom water temperatures on the Iceland shelf, where warmer Atlantic waters converge with southward flowing polar waters, are known to vary significantly on a seasonal to annual time-scale (e.g., Malmberg and Jonsson, 1997).

The sensitivity obtained for *Melonis* species is very similar to sensitivities found in other benthic taxa (Elderfield et al., 2006; Marchitto et al., 2007; Lear et al., 2010; Quillmann et al., 2012), in between the one for the infaunal *Uvigerina* species often used for BWT reconstructions (Elderfield et al., 2006; Bryan and Marchitto, 2008; Elderfield et al., 2010; 2012, Roberts et al., 2016) and species with high Mg content and higher sensitivities, such as *Globobulimina* spp. (Weldeab et al. 2016) and *Hyalinea balthica* (Rosenthal et al., 2011).

5. CONCLUSIONS

Infaunal benthic foraminifera of the genus *Melonis* populate all ocean basins from low to high latitudes, and from the shelf to abyssal depth, and are hence well-suited proxy carriers in paleoceanography. However, existing temperature reconstructions using Mg/Ca ratios of *Melonis* depend upon calibrations that suffer from significant uncertainties. In this study, we have compiled a novel data set, based on new data mostly from the North Atlantic, together with published data. This allows us to establish a Mg/Ca-temperature calibration of high quality extending from -1°C to 16°C described by $\text{Mg/Ca (mmol/mol)} = 0.113 \pm 0.005T + 0.792 \pm 0.036$. Although the limited number of samples with sympatric *Melonis* specimens of varying morphometry makes it difficult to conclusively assess the intra- and interspecific variability of *Melonis*, the relatively small Mg/Ca offsets between sympatric morphotypes suggests that foraminifera of the genus *Melonis* have a similar temperature response. The large deviation between data from the LBB (Lear et al., 2002) and all other data in the compiled data set provides further evidence that *Melonis* tests from the LBB are contaminated

and do not yield Mg/Ca values representative of the original ontogenetic shell. Mg/Ca ratios of the analyzed tests show no strong dependence to bottom water $\Delta[\text{CO}_3^{2-}]$. However, *Melonis* from the tropical eastern Atlantic core top sites that experience high organic carbon flux show lower Mg/Ca than tests from other sites, which might be an indicator of lower pore water $\Delta[\text{CO}_3^{2-}]$ affecting the fractionation of Mg during calcification.

Acknowledgments

We acknowledge the financial support provided by ETH Research Grant ETH-04 11-1 (A.P.H.), and the Swiss National Science Foundation grants PZ00P2_141424 (A.M.-G.) and PP00P2_144811 (S.L.J.). We are very grateful to James Rae, Harry Elderfield, and Mervyn Greaves for making unpublished data available, Karen Louise Knudsen for providing Oslofjord samples, Stéphane Westermann and Corey Archer for support with the solution-based ICP-MS analyses, Antje Sorowka for taking the SEM images at MPIC, and Julia Gottschalk who made the multi-lab collaboration possible.

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1 Table, 6 Figures.

Table 1. Location, bottom water properties, relative abundance, and Mg/Ca of core top *Melonis* presented in this study, ordered by oceanic region and decreasing latitude.

Core ^a	Lat (°N)	Lon (°E)	Depth (m)	BWT ^b (°C)	BWS ^b (psu)	ΔCO_3^{2-} ^c ($\mu\text{mol/kg}$)	Species ^d <i>Melonis</i> ...	Total ^e	Abun. ^f (%)	Mg/Ca ^g (mmol/mol)	Institute/ Cleaning ^h
Nordic Seas											
GIK23004	67.733	5.920	1244	-0.86	34.91	51.9	<i>barl.</i>	881	0.2	0.84	ETHZ - O
GIK23001	67.700	3.832	1257	-0.89	34.91	51.5	<i>barl.</i>	119	0.8	0.77	ETHZ - O
GIK23040	67.003	7.780	967	-0.63	34.91	57.7	<i>barl.</i>	159	2.5	0.79	ETHZ - O
GIK23008	66.932	7.917	840	-0.60	34.92	56.3	<i>barl.</i>	914	3.0	0.69	ETHZ - O
GS19MCA	63.760	5.190	922	-0.72	34.91	74.6	<i>barl.</i>			0.90	CU - O
GIK16119	63.431	3.129	1403	-0.83	34.91	49.0	<i>barl.</i>	211	12.0	0.79	ETHZ - O
GIK16120	63.275	3.210	1205	-0.81	34.91	53.7	<i>barl.</i>	578	15.0	0.78	ETHZ - O
GIK16142	63.152	2.362	1100	-0.83	34.91	55.1	<i>barl.</i>	310	42.0	0.76	ETHZ - O
GIK16121	63.124	3.049	1003	-0.85	34.92	56.8	<i>barl.</i>	304	47.0	0.71	ETHZ - O
GIK16107	63.098	0.343	1497	-0.84	34.91	42.1	<i>barl.</i>	120	2.0	1.05	ETHZ - O
GIK16143	63.093	2.496	1002	-0.79	34.91	57.0	<i>barl.</i>	275	46.0	0.79	ETHZ - O
GIK16144	63.049	2.592	900	-0.76	34.91	53.4	<i>barl.</i>	210	77.0	0.74	ETHZ - O
GIK16122	63.043	3.203	900	-0.80	34.92	53.4	<i>barl.</i>	307	61.0	0.73	ETHZ - O
GIK16106	63.036	0.476	1304	-0.80	34.91	45.2	<i>barl.</i>	198	16.0	0.77	ETHZ - O
KN177-2 MC11	63.032	0.807	1285	-0.80	34.91	45.6	<i>barl.</i>			0.91	CU - R
GS04-138-21	62.860	-6.130	652	-0.24	34.91	82.0	<i>barl.</i>			1.00	INSTAAR - R
GIK15MCA ³	62.860	-6.11	592	-0.14	34.90	90.8	<i>barl.</i>			0.98	CU - O
GS16MCA	62.840	-6.17	550	0.04	34.90	92.2	<i>barl.</i>			1.05	CU - O
KN177-2 MC14	62.819	1.300	965	-0.74	34.91	55.8	<i>barl.</i>			0.89	CU - R
KN177-2 MC6	62.604	1.744	695	-0.47	34.91	57.0	<i>barl.</i>			0.83	CU - R
GIK16145	62.590	3.141	803	-0.65	34.92	53.8	<i>barl.</i>	211	56.0	0.73	ETHZ - O
GIK16105	62.566	1.020	1100	-0.80	34.91	55.1	<i>barl.</i>	365	8.0	0.68	ETHZ - O
GIK16123	62.529	3.427	801	-0.70	34.92	53.8	<i>barl.</i>	394	78.0	0.76	ETHZ - O
GIK16146	62.516	3.300	693	-0.74	34.91	56.8	<i>barl.</i>	99	35.0	0.74	ETHZ - O
GIK16124	62.468	3.537	605	-0.35	34.91	60.4	<i>barl.</i>	294	26.0	0.96	ETHZ - O
GIK16147	62.462	3.431	607	-0.32	34.91	60.3	<i>barl.</i>	156	54.0	0.89	ETHZ - O
GIK16149	62.410	3.536	401	5.46	35.10	75.1	<i>barl.</i>	205	1.0	1.52	ETHZ - O
MC56E	62.402	3.137	380	2.77	34.98	90.3	<i>barl.</i>			1.35	CU - O
GIK16150	62.390	3.591	293	7.15	35.21	84.4	<i>barl.</i>	229	1.0	1.84	ETHZ - O
GIK16151	62.380	4.002	205	7.85	35.25	87.3	<i>barl.</i>	110	1.0	1.77	ETHZ - O
GIK16104	62.369	1.434	702	-0.49	34.91	73.8	<i>barl.</i>	394	56.0	0.77	ETHZ - O
GIK16152	62.183	4.396	144	8.09	35.21	88.7	<i>barl.</i>	294	6.0	2.05	ETHZ - O
KN177-2 MC4	62.120	2.721	418	5.15	35.08	73.6	<i>barl.</i>			1.21	CU - R
GIK16103	62.074	2.432	410	5.70	35.09	75.0	<i>barl.</i>	248	17.0	1.18	ETHZ - O
Oslofjord (Risdal, 1964)											
Station 35	59.650	10.617	100	7.20	34.90	74.0	<i>barl.</i>			2.03	INSTAAR - R
Station 21	59.333	10.617	220	6.66	35.14		<i>barl.</i>			2.00	INSTAAR - R
Station 20	59.317	10.550	155	6.88	35.07	78.8	<i>barl.</i>			1.79	INSTAAR - R
Station 11 ²	59.283	10.650	50	8.03	34.36	64.1	<i>barl.</i>			2.16	INSTAAR - R
Station 11 ²	59.283	10.650	50	8.03	34.36	64.1	<i>barl. fat</i>			3.43	INSTAAR - R
Station 6	59.267	10.658	105	7.17	34.92	74.2	<i>barl.</i>			1.63	INSTAAR - R
Station 6	59.267	10.658	105	7.17	34.92	74.2	<i>barl. fat</i>			1.53	INSTAAR - R
Subtropical to northern North Atlantic											
RapiD-10-1P	62.976	-15.590	1237	4.47	35.00	66.3	<i>barl.</i>			1.51	GLPR - O
RapiD-4-2C	61.739	-15.402	2284	3.08	34.97	46.9	<i>barl.</i>			1.39	GLPR - O
RapiD-17-5P	61.482	-19.536	2303	2.95	34.99	36.8	<i>barl.</i>			1.30	CU - O
GIK16202	60.475	-8.744	330	8.77	35.32	98.7	<i>barl.</i>	96	10.4	1.35	ETHZ - O
GIK16205	60.332	-12.628	305	8.58	35.27	100.7	<i>barl.</i>	31	29.0	2.02	ETHZ - O
GIK16204	60.139	-13.358	609	8.13	35.25	96.3	<i>barl.</i>	33	6.1	1.82	ETHZ - O
GIK16201	59.601	-7.714	904	7.26	35.27	84.6	<i>barl.</i>	155	0.6	1.69	ETHZ - O
RapiD-32-22B	58.249	-47.012	3096	2.08	34.91	34.3	<i>barl.</i>			1.18	CU - O
RapiD-35-25B	57.508	-48.723	3486	1.80	34.90	28.0	<i>barl.</i>			1.10	CU - O
GIK16213	57.158	-13.019	1207	5.66	35.10	72.6	<i>barl.</i>	173	2.9	1.38	ETHZ - O
GIK16214	57.105	-13.200	638	8.86	35.32	89.5	<i>barl.</i>	196	1.0	1.98	ETHZ - O
GIK16220	52.699	-14.868	709	9.54	35.37	68.4	<i>barl.</i>	142	1.4	1.79	ETHZ - O
GIK16901	49.285	-11.416	410	10.95	35.53	95.2	<i>barl. mix</i>	268	2.2	2.25	ETHZ - O
GIK16901	49.285	-11.416	410	10.95	35.53	95.2	<i>barl. fat</i>			2.09	ETHZ - O
GIK16906	49.010	-13.567	3889	2.51	34.91	12.3	<i>barl.</i>	171	2.9	1.18	ETHZ - O
GIK16906	49.010	-13.567	3889	2.51	34.91	12.3	<i>pomp.</i>	171	0.0	1.05	ETHZ - O
GIK10792	40.500	-9.655	1268	10.38	36.11	86.8	<i>barl.</i>	65	2.0	1.88	ETHZ - O
GIK10809	40.325	-9.572	182	12.82	35.78	111.0	<i>barl.</i>	363	1.1	2.39	ETHZ - O
GIK10810	40.325	-9.452	146	13.16	35.83	114.6	<i>barl. mix</i>	386	0.8	2.34	ETHZ - O
GIK10802 ⁴	40.303	-9.785	816	11.53	36.09	82.5	<i>barl.</i>	385	1.6	3.63	ETHZ - O

GIK10808	40.303	-9.618	211	12.60	35.75	108.0	barl.	251	4.8	2.27	ETHZ - O
GIK10805	40.292	-9.667	377	11.59	35.61	93.0	barl.	115	2.6	1.99	ETHZ - O
GIK10801	40.280	-9.845	1010	11.22	36.15	83.3	barl.	103	3.9	1.81	ETHZ - O
GIK10807	40.280	-9.632	238	12.42	35.72	105.3	barl. mix	35	4.0	2.18	ETHZ - O
GIK10806	40.270	-9.643	287	12.05	35.66	100.8	barl.	217	6.5	1.96	ETHZ - O
GIK10770	37.708	-9.375	618	12.12	36.01	83.9	barl.	406	18.5	2.13	ETHZ - O
GIK8060	37.692	-9.500	996	11.59	36.28	73.6	barl.	104	6.7	2.19	ETHZ - O
GIK8060	37.692	-9.500	996	11.59	36.28	73.6	barl. fat			2.26	ETHZ - O
GIK8011	37.689	-9.255	500	11.78	35.77	87.5	barl.	204	9.3	1.90	ETHZ - O
GIK10769	37.683	-9.475	611	12.10	36.00	83.9	barl.	70	2.8	2.65	ETHZ - O
GIK10767	37.675	-9.717	1709	6.41	35.45	49.9	barl.	165	1.8	1.61	ETHZ - O
GIK10777	37.638	-8.973	148	14.34	36.02	121.5	barl. mix	610	1.0	2.59	ETHZ - O
GIK10774	37.612	-9.283	600	12.07	35.97	84.0	barl. fat	214	7.0	2.26	ETHZ - O
GIK15809	35.962	-7.314	945	10.40	35.87	69.0	barl. fat	131	1.5	2.12	ETHZ - O
GIK15659 ²	34.893	-6.758	285	13.43	35.86	104.2	barl. mix	37	2.7	2.56	ETHZ - O
GIK15658	34.887	-6.703	205	14.46	36.11	114.0	barl.	289	0.7	2.33	ETHZ - O
GIK15653	34.870	-6.602	140	15.43	36.25	115.6	barl.	146	0.7	2.33	ETHZ - O
GIK15652	34.868	-6.582	130	15.58	36.26	115.5	barl.	101	2.0	2.47	ETHZ - O
GIK15678	33.472	-12.750	4305	2.46	34.90	-1.9	pomp.	156	*1.1	0.98	ETHZ - O
GIK15644 ⁴	32.398	-9.808	485	11.76	35.63	81.5	barl.	86	1.2	3.64	ETHZ - O
GIK15644	32.398	-9.808	485	11.76	35.63	81.5	barl. fat			2.78	ETHZ - O
GIK15645 ⁴	32.383	-9.783	440	12.13	35.68	86.0	barl.	99	*3.3	3.66	ETHZ - O
GIK15645 ⁴	32.383	-9.783	440	12.13	35.68	86.0	barl. fat			3.26	ETHZ - O
GIK16005	29.247	-11.507	811	9.18	35.42	47.2	barl.			1.87	ETHZ - O
GIK16005	29.247	-11.507	811	9.18	35.42	47.2	barl. fat			1.89	ETHZ - O
GIK15634	28.255	-13.395	1215	6.70	35.27	39.0	barl. fat	353	0.8	1.84	ETHZ - O
GIK15635	27.203	-14.660	2605	3.10	34.97	25.4	pomp.	306	*0.7	1.07	ETHZ - O
GIK12306	26.327	-14.928	741	6.59	35.27	42.4	barl.	65	3.1	1.83	ETHZ - O
Tropical North Atlantic											
GIK12328	21.145	-18.573	2822	2.78	34.95	17.3	barl.	94	5.3	0.85	ETHZ - O
GIK12328	21.145	-18.573	2822	2.78	34.95	17.3	pomp.	94	2.1	0.91	ETHZ - O
GIK13533	20.993	-18.032	2112	3.46	34.99	26.0	barl.	115	14.8	1.02	ETHZ - O
GIK13533	20.993	-18.032	2112	3.46	34.99	26.0	pomp.	115	0.9	0.99	ETHZ - O
GIK12347	15.825	-17.845	2710	2.88	34.94	24.7	barl.	133	3.8	0.80	ETHZ - O
GIK12347	15.825	-17.845	2710	2.88	34.94	24.7	pomp.	133	2.3	0.92	ETHZ - O
GIK12346	15.570	-17.545	1517	4.38	34.97	29.0	barl.	171	*0.5	0.86	ETHZ - O
GIK13237	14.118	-17.640	996	5.80	34.87	32.5	barl.	334	8.4	1.13	ETHZ - O
GIK13238	14.097	-17.875	1983	3.52	34.97	29.6	barl.	286	10.1	0.94	ETHZ - O
GIK13238	14.097	-17.875	1983	3.52	34.97	29.6	pomp.	286	0.0	0.54	ETHZ - O
GIK16420	9.928	-17.533	806	5.84	34.70	10.8	barl.	100	3.0	1.05	ETHZ - O
GIK16753	9.583	-16.543	457	8.95	34.97	16.6	barl.	189	4.8	1.61	ETHZ - O
GIK16754	9.503	-16.623	646	6.79	34.73	10.0	barl.	149	1.3	1.17	ETHZ - O
GIK16755	9.253	-16.858	1002	5.12	34.75	31.2	barl.	195	1.0	1.05	ETHZ - O
GIK16762	8.395	-14.413	302	11.49	35.17	34.0	barl.	105	1.0	2.74	ETHZ - O
GIK16850 ⁴	6.102	3.670	247	12.39	35.23	45.6	barl.	133	3.8	3.60	ETHZ - O
GIK16852	6.072	3.643	770	5.23	34.55	20.0	barl.	199	1.5	0.97	ETHZ - O
GIK16853	6.065	3.642	1018	4.56	34.67	62.3	barl.	153	4.6	0.94	ETHZ - O
GIK16844 ¹	5.720	1.160	1230	4.43	34.86	69.3	barl.	252	0.8	0.90	ETHZ - O
GIK16845 ¹	5.557	1.150	2007	3.50	34.95	74.8	barl.	192	3.6	0.68	ETHZ - O
GIK16846	5.365	1.287	2739	2.90	34.92	56.6	barl.	239	1.3	0.75	ETHZ - O
GIK16813	5.008	-4.547	297	10.83	35.04	36.5	barl. fat	132	2.3	2.22	ETHZ - O
GIK16806	4.950	-4.553	1204	4.45	34.81	62.5	barl.	183	4.4	0.96	ETHZ - O
GIK16801	4.520	-6.473	310	10.56	35.01	34.1	barl.	164	0.6	2.01	ETHZ - O
GIK16786	4.512	-9.147	451	7.98	34.75	30.5	barl.	110	8.2	1.87	ETHZ - O
GIK16820	4.503	-2.303	445	8.06	34.76	17.0	barl.	190	5.8	1.45	ETHZ - O
GIK16787	4.482	-9.195	674	5.90	34.60	24.9	barl.	152	3.3	1.05	ETHZ - O
GIK16819	4.453	-2.335	631	6.12	34.60	13.5	barl.	150	6.0	1.09	ETHZ - O
GIK16799	4.447	-6.433	1505	4.11	34.94	43.1	barl.	154	4.5	0.91	ETHZ - O
GIK16818	4.388	-2.367	749	5.34	34.56	12.9	barl.	177	1.1	0.94	ETHZ - O
GIK16831	4.350	-1.152	632	6.02	34.58	13.3	barl.	132	1.5	1.36	ETHZ - O
GIK16798	4.345	-6.402	2221	3.20	34.95	42.4	barl.	138	0.7	0.74	ETHZ - O
GIK16817	4.322	-2.383	1001	4.56	34.65	25.0	barl.	158	1.3	0.91	ETHZ - O
GIK16796	4.101	-6.268	3296	2.52	34.90	23.1	pomp.	256	0.0	0.81	ETHZ - O
GIK16861	3.622	6.500	403	8.74	34.78	26.3	barl.	123	3.3	1.29	ETHZ - O
GIK16862	3.547	6.487	698	5.54	34.55	27.5	barl.	167	3.6	0.96	ETHZ - O
GIK16863	3.397	6.415	993	4.57	34.65	60.4	barl.	165	1.2	0.88	ETHZ - O
Eastern South Atlantic											
GeoB12808-4	-26.370	11.892	3796	1.79	34.82	21.2	barl.			1.20	UoB - O
Sulawesi margins											
BJ8-03MC24	-5.065	117.448	832	5.18	34.55	2.5	barl.			1.41	CU - R
BJ8-03MC29	-3.894	119.370	987	4.72	34.56	15.1	barl.			1.56	CU - R
BJ8-03MC22	-3.887	119.495	1189	4.13	34.57	10.9	barl.			1.90	CU - R
Pacific Southern Ocean											
PS75/073-2	-57.204	-151.611	3234	0.77	34.71	2.5	pomp.			0.82	ETHZ - O

^a Rejected samples have a superscript next to their core name: 1 = high Fe/Ca and/or Fe/Mg; 2 = high Mn/Ca; 3 = high Al/Ca; 4 = outlier ($>2\sigma$).

^b Temperature (Locarnini et al., 2013) and salinity (Zweng et al., 2013) data are from WOA13.

^c Calculation of ΔCO_3^{2-} is explained in detail in the text.

^d The abbreviations 'barl.' and 'pomp.' stands for *barleeaanum* and *pompilioides*. The different morphotypes of *M. barleeaanum* are distinguished: 'barl.' = compressed to transitional; 'barl. fat' = spherical; 'barl. mix' = compressed to spherical.

^e Total sum of counted benthic specimens in the $>250\ \mu\text{m}$ fraction (Seiler, 1975; Haake, 1980; Lutze and Coulbourn, 1984; Mackensen et al., 1985; Thies, 1991; Timm, 1992; Schiebel, 1992; Altenbach et al., 1999; Altenbach et al. 2003; Schönfeld and Altenbach, 2005).

^f Abundance of living *M. barleeaanum* (all morphotypes) and *M. pompilioides* relative to all benthic foraminifera species in the $>250\ \mu\text{m}$ fraction. The asteriks mark samples where the relative abundance was determined on the dead assemblage. See reference in ^e.

^g Mg/Ca values of samples cleaned reductively are corrected (increased) by factor 1.10 (Yu et al., 2007).

^h Samples were processed at {ETHZ = ETH Zurich; GLPR = University of Cambridge; INSTAAR = University of Colorado; CU = Cardiff University; UoB = University of Bristol} using {O = oxidative cleaning; R = oxidative and reductive cleaning}.

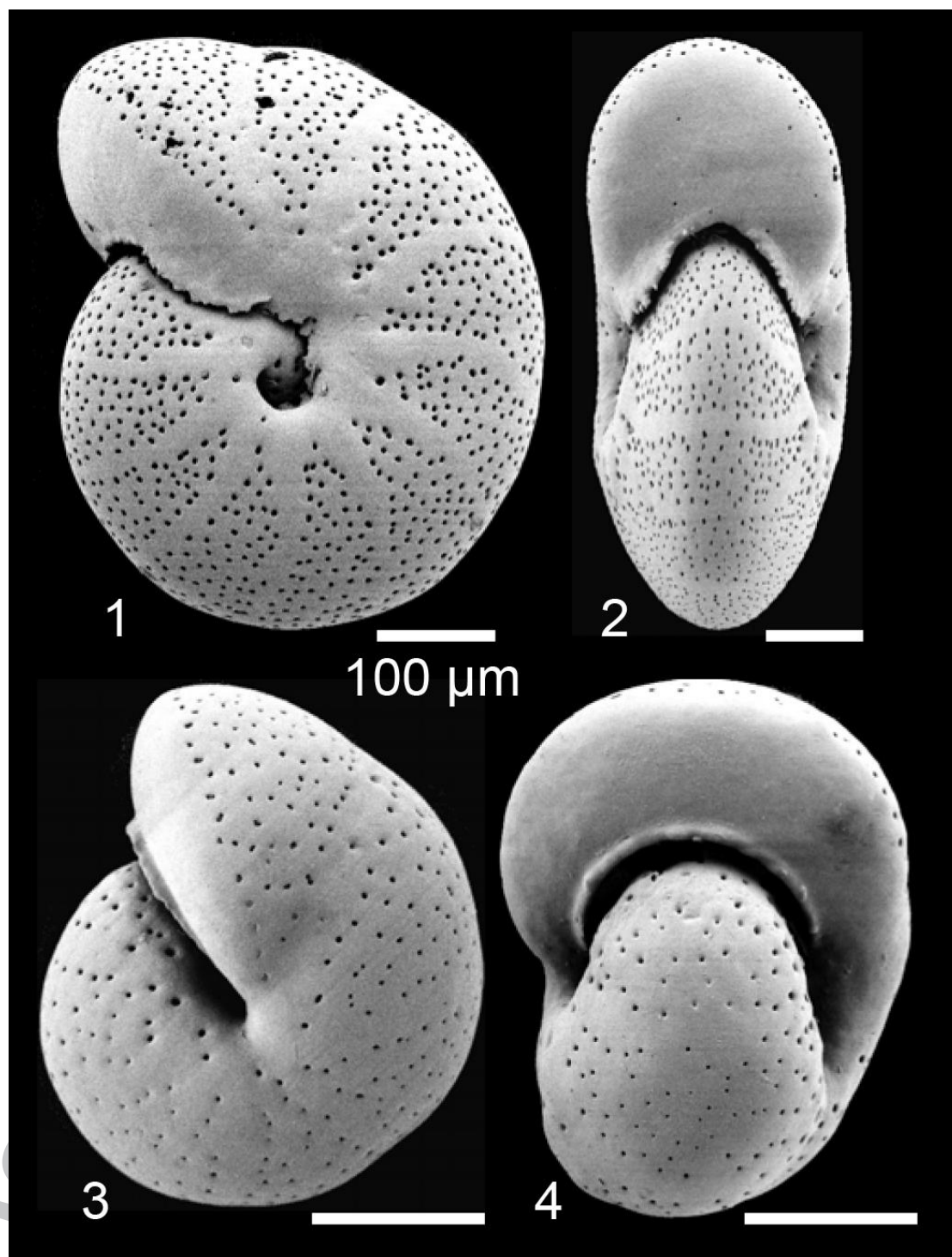


Figure 1. *Melonis barleeaanum* (1, 2) and *Melonis pompilioides* (3, 4) in lateral (1, 3) and frontal (2, 4) view. Both specimens are from sediments of ODP Site 1094 (77.55 mcd). All scale bars are 100 µm.

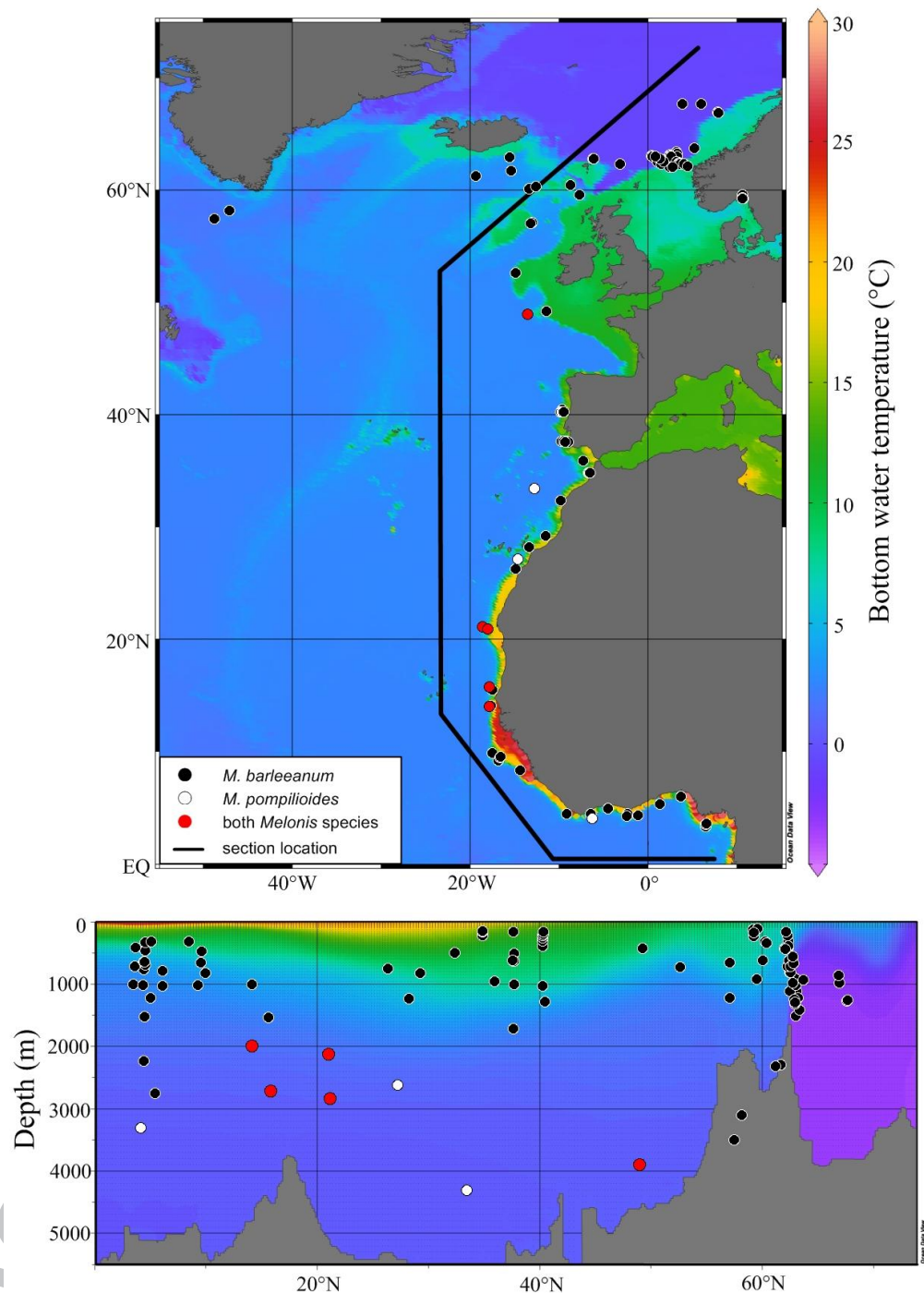


Figure 2. Locations of North Atlantic core top samples investigated in this study shown on a surface map and a latitudinal transect depicting bottom water temperature. Sample locations cover a large range of oceanographic conditions in the North Atlantic spanning -0.9°C (Norwegian Sea) to 15.6°C (shallow site off Morocco). In addition to the sites shown on the map, three core tops from the Sulawesi margin, one core top from the South Atlantic and one core top from the Pacific Southern Ocean were analyzed (see Table 1).

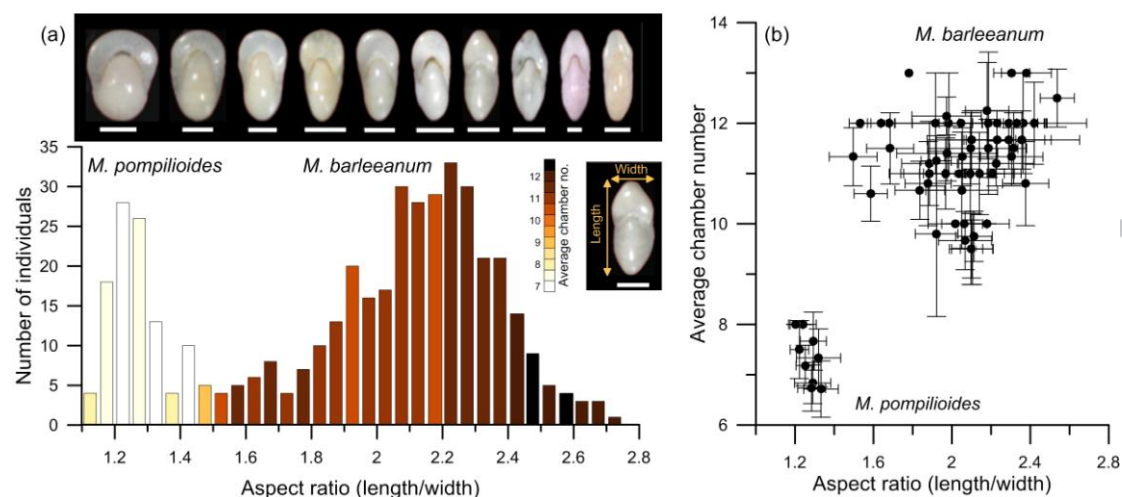


Figure 3. (a) Histogram of the aspect ratio (length/width) of the *Melonis* specimens processed at ETHZ/MPIC (black symbols in Fig. 4a) showing two peaks centered around 2.2 (*M. barleeaanum*) and 1.25 (*M. pompilioides*), respectively. The average chamber number, spanning between 7 (pale yellow) and 13 (dark red), varies with the aspect ratio. At the top, characteristic *Melonis* morphotypes are depicted in frontal view with their aspect ratio roughly corresponding to the x-axis below (from left to right: GIK13533, GIK15809, GIK10774, GIK10774, GIK10774, GIK16119, GIK10774, GIK16861, GIK16853, GIK13533). Note that the second test from the right is Rose Bengal stained. (b) Relationship between aspect ratio and chamber number for the core tops investigated. All scale bars are 200 μm .

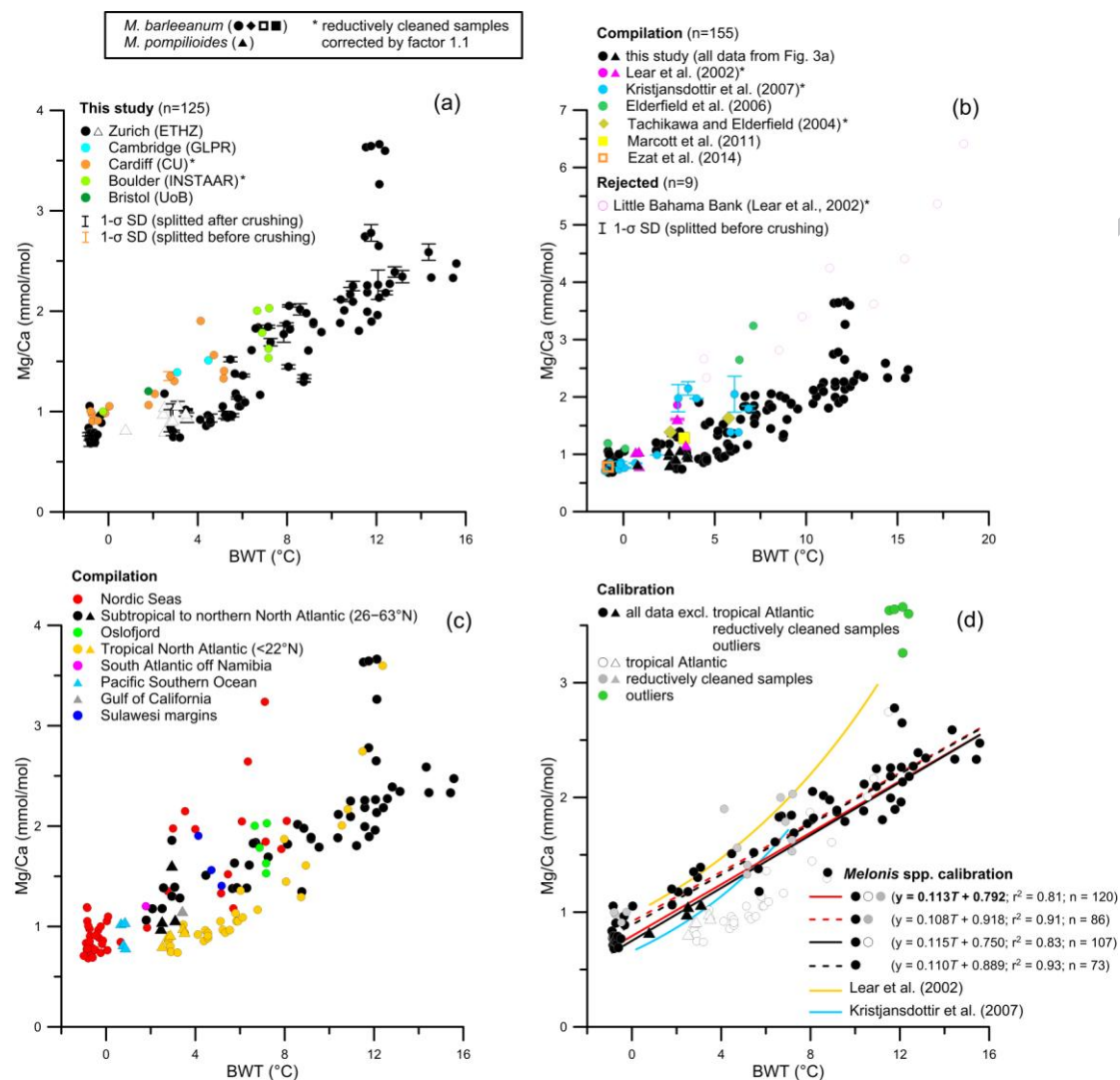


Figure 4. Relationship between bottom water temperature (°C; BWT) and Mg/Ca ratio of *Melonis* (mmol/mol). *Melonis pompilioides* are shown as triangles throughout. Reductively cleaned samples are corrected by factor 1.10 (Yu et al., 2007). (a) Mg/Ca analyses from this study. The SD of the samples processed at CU (orange) and ETHZ (black) include samples, which were split before and after crushing, respectively. (b) Compilation of new and published *Melonis* Mg/Ca ratios. The previously published data from the Little Bahama Bank (Lear et al., 2002) were rejected (open pink circles). (c) Mg/Ca data shown in (b) plotted with the color code labeling the different oceanic regions. (d) Mg/Ca data shown in (a), and differentiating between the tropical Atlantic and all other data, as well as on the cleaning method. The calibration curves only include data newly presented in this study. They are based on the entire data set (red solid line), and on all data excluding the tropical Atlantic data

(red dashed line), excluding the reductively cleaned samples (black solid line), and excluding both the tropical Atlantic data and reductively cleaned samples (black dashed line). Also shown are the five outliers in green, and the previously published calibration curves, not corrected for the cleaning method (Lear et al., 2002; Kristjansdottir et al., 2007).

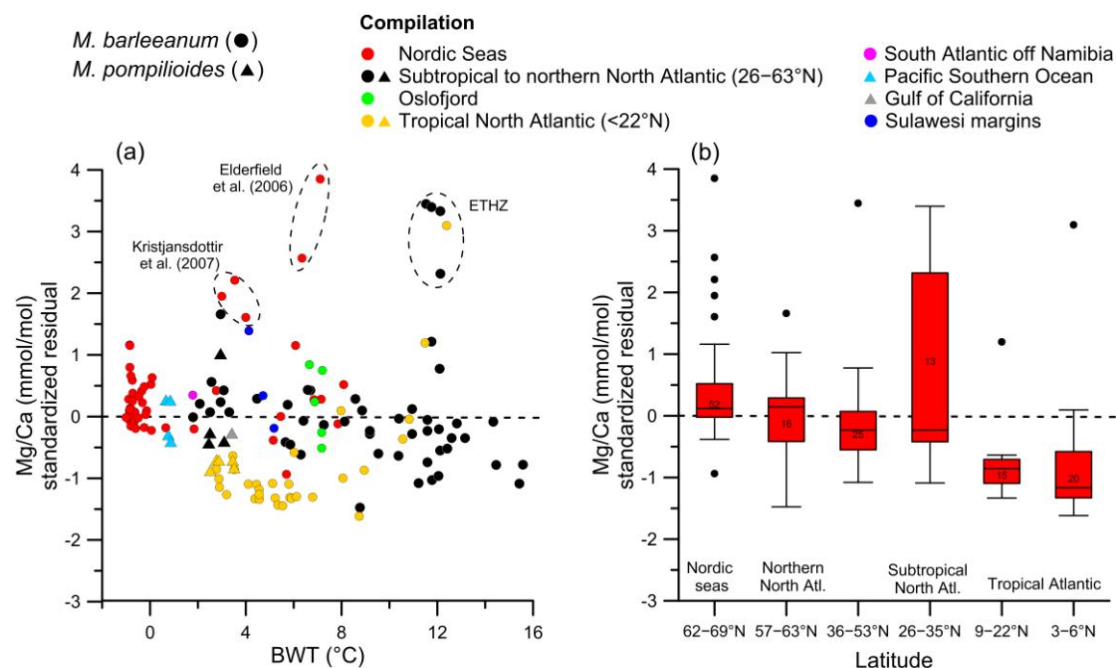


Figure 5. (a) Standardized Mg/Ca residuals of all data shown in Fig. 3b (except for LBB), calculated by removing the temperature trend. (b) Mg/Ca residuals of the North Atlantic grouped into six latitudinal regions. The box whisker plots emphasize the discrepancy between the tropical North Atlantic data and the extratropical North Atlantic data.

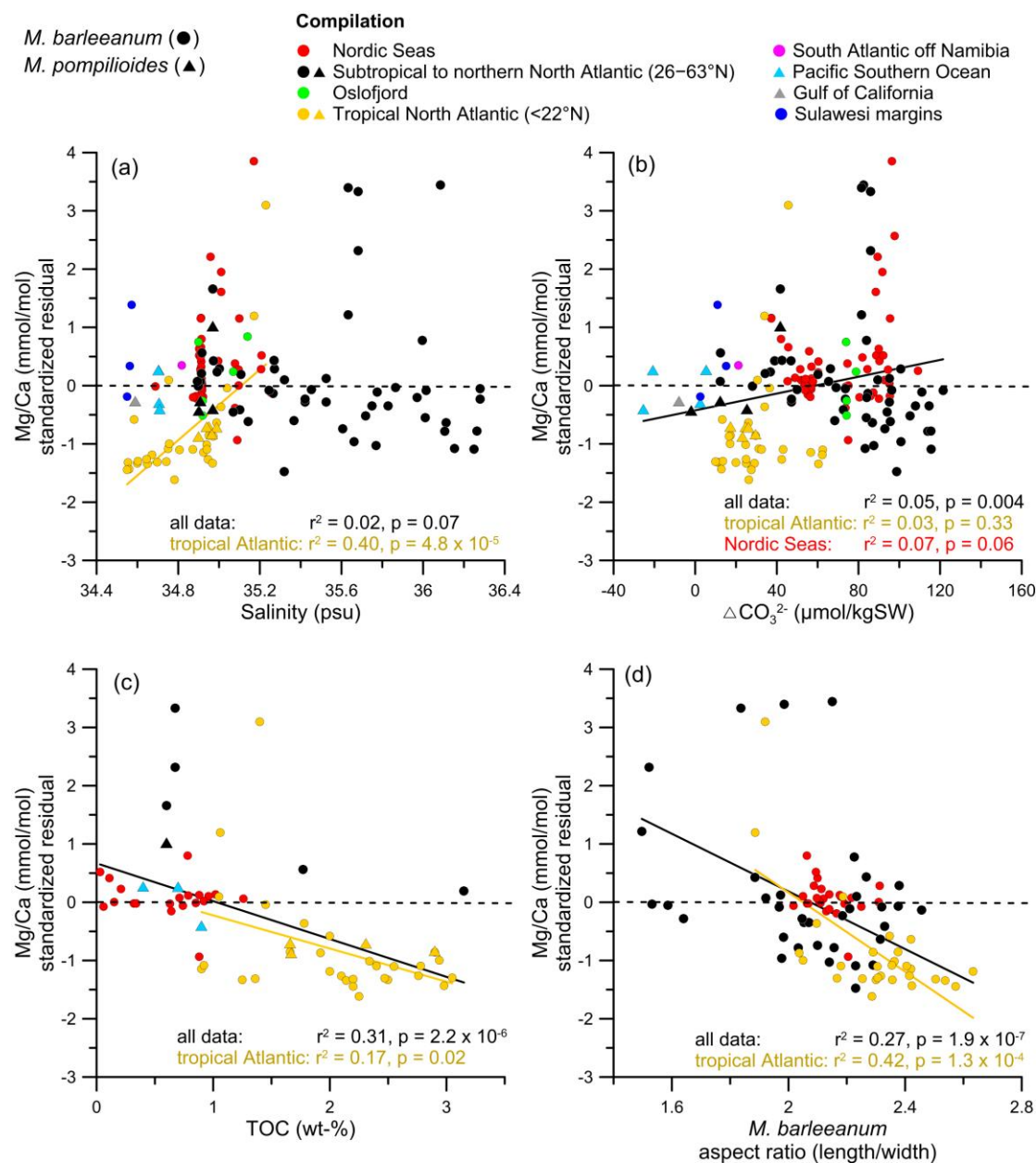


Figure 6. Standardized Mg/Ca residuals compared to (a) salinity, (b) $\Delta[\text{CO}_3^{2-}]$, (c) TOC, and (d) the aspect ratio of *M. barleeaanum*. The linear fits are only shown when the correlation is significant ($p < 0.05$).